Diethyl propanedioate
105-53-3 | DTXSID7021863

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 21.4 L/kg

Global applicability domain: Inside

Local applicability domain index: 4.90e-01

Confidence level: 5.99e-01

Nearest Neighbors from the Training Set

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N-Methyl-N'-phenylurea
Measured: 19.5
Predicted: 29.8

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Urea, 1-(p-fluorophenyl)-
Measured: 33.1
Predicted: 49.6

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1-Methoxy-2-propyl acetate
Measured: 2.29
Predicted: 7.33

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Urea, (3-methylphenyl)-
Measured: 36.3
Predicted: 37.2

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N-(3-chlorophenyl)-N'-
methylurea
Measured: 85.1
Predicted: 101